```
C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\112rtl.str
chain nodes :
                                         34
                                             35
                                                 37
                                                                 44
    10 11 12
               19
                   20
                        21
                            22
                                23
                                     25
ring nodes :
                                                                    31
                                                                        32
                                                                            33
                                                            29
                                                                30
    1 2 3
                      7
                         8
                            9 13 14
                                       15
                                            16
                                                17
                                                    18
                                                        28
chain bonds :
    1-11 6-10 7-12 11-41 12-15 13-21
                                                   16-19 17-23
                                                                 18-22
                                                                        32 - 34
                                            14-20
    34-35 42-43 42-44
```

```
ring bonds :
    1-2 1-4 2-3 3-6 4-5
                            5-9 6-7 7-8
                                          8-9 13-14 13-18 14-15
    16-17 17-18 28-29 28-33 29-30
                                      30-31 31-32 32-33
exact/norm bonds :
    1-11 6-10 11-41 34-35 42-43 42-44
exact bonds :
    1-2 1-4 2-3 3-6 4-5 5-9 6-7 7-8 7-12 8-9 12-15
                                                              13-21
    16-19 17-23 18-22 32-34
normalized bonds :
                                                            29-30 30-31 31-32
   13-14 13-18 14-15
                        15-16 16-17 17-18 28-29 28-33
    32 - 33
isolated ring systems :
    containing 1 : 13 : 28 :
G1:CH3,Et
G2:H,[*1],[*2]
Match level:
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom
                                                   7:Atom 8:Atom 9:Atom
    10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 25:CLASS
                                                   15:Atom 16:Atom 17:Atom
            28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:CLASS
             37:Atom 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:Atom
    35:CLASS
Generic attributes :
    37:
```

Saturation

: Unsaturated

Element Count : Node 37: Limited N,N2 C,C7

```
=> d his
     (FILE 'HOME' ENTERED AT 14:26:42 ON 21 MAR 2007)
     FILE 'REGISTRY' ENTERED AT 14:26:53 ON 21 MAR 2007
                 STRUCTURE UPLOADED
L1
              14 S L1
L2
             277 S L1 FULL
L3
     FILE 'HCAPLUS' ENTERED AT 14:39:46 ON 21 MAR 2007
              25 S L3
L4
              4 S L4 AND SAKANAKA, O?/AU
L5
              21 S L4 NOT L5
L6
               0 S L6 AND MITOMO, K?/AU
L7
               0 S L6 AND TAMURA, T?/AU
0 S L6 AND MURAJ, Y?/AU
^{\text{L8}}
L9
               0 S L6 AND IINUMA, K?/AU
L10
               0 S L6 AND TERAOKA, T?/AU
L11
               0 S L6 AND KUZUHARA, K?/AU
L12
              0 S L6 AND MIKOSHIBA, H?/AU
L13
              12 S L6 AND TANIGUCHI, M?/AU
L14
     FILE 'CAOLD' ENTERED AT 14:46:48 ON 21 MAR 2007
=> s 13
```

0 L3 L15

=>

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```
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      1
                  "Ask CAS" for self-help around the clock
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 NEWS
                  CA/CAplus pre-1967 chemical substance index entries enhanced
         DEC 18
 NEWS
                  with preparation role
                  CA/CAplus patent kind codes updated
      4
          DEC 18
 NEWS
                  MARPAT to CA/CAplus accession number crossover limit increased
          DEC 18
 NEWS
      5
                  to 50,000
                  MEDLINE updated in preparation for 2007 reload
          DEC 18
 NEWS
       6
          DEC 27
                  CA/CAplus enhanced with more pre-1907 records
 NEWS
      7
          JAN 08
                  CHEMLIST enhanced with New Zealand Inventory of Chemicals
 NEWS
      8
                  CA/CAplus Company Name Thesaurus enhanced and reloaded
      9
          JAN 16
 NEWS
                  IPC version 2007.01 thesaurus available on STN
          JAN 16
 NEWS 10
 NEWS 11
                  WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
          JAN 16
 NEWS 12
          JAN 22
                  CA/CAplus updated with revised CAS roles
 NEWS 13
                  CA/CAplus enhanced with patent applications from India
          JAN 22
                  PHAR reloaded with new search and display fields
 NEWS 14
          JAN 29
                  CAS Registry Number crossover limit increased to 300,000 in
 NEWS 15
          JAN 29
                  multiple databases
 NEWS 16
          FEB 15
                  PATDPASPC enhanced with Drug Approval numbers
 NEWS 17
          FEB 15
                  RUSSIAPAT enhanced with pre-1994 records
                  KOREAPAT enhanced with IPC 8 features and functionality
          FEB 23
 NEWS 18
          FEB 26
                  MEDLINE reloaded with enhancements
 NEWS 19
                  EMBASE enhanced with Clinical Trial Number field
          FEB 26
 NEWS 20
          FEB 26
                  TOXCENTER enhanced with reloaded MEDLINE
 NEWS 21
 NEWS 22
          FEB 26
                  IFICDB/IFIPAT/IFIUDB reloaded with enhancements
                  CAS Registry Number crossover limit increased from 10,000
 NEWS 23
          FEB 26
                  to 300,000 in multiple databases
          MAR 15
                  WPIDS/WPIX enhanced with new FRAGHITSTR display format
 NEWS 24
 NEWS 25
          MAR 16
                  CASREACT coverage extended
 NEWS 26
          MAR 20
                  MARPAT now updated daily
 NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
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SINCE FILE TOTAL
ENTRY SESSION
0.21 0.21

FULL ESTIMATED COST

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New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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http://www.cas.org/ONLINE/UG/regprops.html

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L1 STRUCTURE UPLOADED

=> s 11

SAMPLE SEARCH INITIATED 14:39:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 23 TO ITERATE

100.0% PROCESSED SEARCH TIME: 00.00.01 23 ITERATIONS

14 ANSWERS

JERMON TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

14 SEA SSS SAM L1

PROJECTED ITERATIONS: 173 TO 747
PROJECTED ANSWERS: 56 TO 504

·

Updated Search

=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:39:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 477 TO ITERATE

100.0% PROCESSED 477 ITERATIONS 277 ANSWERS

SEARCH TIME: 00.00.01

L3 277 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS

SINCE FILE
ENTRY
ENTRY
SESSION
FULL ESTIMATED COST

181.31

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 25 L3

=> s 14 and sakanaka, o?/au 25 SAKANAKA, O?/AU L5 4 L4 AND SAKANAKA, O?/AU

=> d 15, ibib abs hitstr, 1-4

L5 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2005:286346 HCAPLUS

DOCUMENT NUMBER:

143:315

TITLE:

Semi-synthesis and biological evaluation of analogues

of UK-2A, a novel antifungal antibiotic from

Streptomyces sp. 517-02

AUTHOR(S):

Usuki, Yoshinosuke; Mitomo, Koichi; Adachi, Noriko;

Ping, Xu; Fujita, Ken-Ichi; Sakanaka, Osamu; Iinuma, Katsuharu; Iio, Hideo; Taniguchi, Makoto

CORPORATE SOURCE: Department of Material Science, Graduate School of

Science, Osaka City University, Sumiyoshi-ku, Osaka,

558-8585, Japan

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),

15(8), 2011-2014

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:315

AB Several analogs of UK-2A, a novel antifungal antibiotic isolated from Streptomyces sp. 517-02, were semi-synthesized for structure-activity studies. In vitro antifungal activities of these compds. against Saccharomyces cerevisiae IFO 0203 were evaluated by the conventional paper disk method. Several derivs. exhibited growth inhibitory activity similar

to UK-2A. IT 234112-93-7P 234113-05-4P

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(semi-synthesis and antifungal antibiotic activity of analogs of UK-2A from Streptomyces sp. 517-02)

RN 234112-93-7 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[3-(acetyloxy)-4-methoxy-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-05-4 HCAPLUS

CN Heptanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl phenylmethyl ester (9CI) (CA INDEX NAME)

IT 167173-85-5, UK-2A

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(semi-synthesis and antifungal antibiotic activity of analogs of UK-2A from Streptomyces sp. 517-02)

RN 167173-85-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 186528-19-8P 215798-04-2P 234112-79-9P

234112-83-5P 234112-92-6P 234113-08-7P

234113-13-4P 234113-22-5P 852473-21-3P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(semi-synthesis and antifungal antibiotic activity of analogs of UK-2A from Streptomyces sp. 517-02)

RN 186528-19-8 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3,4-dimethoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 215798-04-2 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 234112-79-9 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(1,2-dihydro-2-oxo-3-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-83-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3,4-dihydro-3-oxo-2-quinoxalinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-92-6 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-6-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

234113-08-7 HCAPLUS RN

Heptanedioic acid, mono[4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-CN 1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

234113-13-4 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxybenzoyl)amino]-6-CN methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

234113-22-5 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(dimethylamino)-2-CN hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-(CA INDEX NAME) yl ester (9CI)

Absolute stereochemistry.

Updated Search

RN 852473-21-3 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[3-(2-ethoxy-2-oxoethoxy)-4-methoxy-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 234112-77-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(semi-synthesis and antifungal antibiotic activity of analogs of UK-2A from Streptomyces sp. 517-02)

RN 234112-77-7 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 210300-07-5 CMF C19 H25 N O6

2 CM

CRN 104-15-4 CMF C7 H8 O3 S

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS 13 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN L5

ACCESSION NUMBER:

1999:511149 HCAPLUS

DOCUMENT NUMBER:

131:129825

TITLE:

Novel antifungal compounds and process for producing

the same

INVENTOR(S):

Sakanaka, Osamu; Teraoka, Takeshi; Mitomo,

Koichi; Tamura, Takayoshi; Murai, Yasushi; Iinuma, Katsuharu; Kuzuhara, Kikuko; Mikoshiba, Haruki; Taniguchi, Makoto

PATENT ASSIGNEE(S):

Meiji Seika Kaisha, Ltd., Japan

SOURCE:

PCT Int. Appl., 92 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PA'    | PATENT NO.          |     |     |             |             | KIND DATE |                |                 | APPLICATION NO. |      |      |          |     | DATE     |     |      |     |
|--------|---------------------|-----|-----|-------------|-------------|-----------|----------------|-----------------|-----------------|------|------|----------|-----|----------|-----|------|-----|
| WO.    | 9940081             |     |     |             |             |           | 19990812       |                 | WO 1999-JP541   |      |      |          |     | 19990208 |     |      |     |
|        |                     |     |     |             |             |           | BA,            |                 |                 |      |      |          |     |          |     |      |     |
|        |                     | DK, | EE, | ES,         | FI,         | GB,       | GD,            | GE,             | GH,             | GM,  | HR,  | HU,      | ID, | IL,      | IN, | IS,  | JP, |
|        |                     |     |     |             |             |           | LC,            |                 |                 |      |      |          |     |          |     |      |     |
|        |                     |     |     |             |             |           | PT,            |                 |                 |      |      |          |     |          |     |      |     |
|        |                     | TR, | TT, | UA,         | UG,         | US,       | UZ,            | VN,             | YU,             | zw   |      |          |     |          |     |      |     |
|        | RW:                 | GH, | GM, | ΚE,         | LS,         | MW,       | SD,            | SZ,             | UG,             | ZW,  | ΑT,  | BE,      | CH, | CY,      | DE, | DK,  | ES, |
|        |                     | FI, | FR, | GB,         | GR,         | IE,       | IT,            | LU,             | MC,             | NL,  | PT,  | SE,      | BF, | ВJ,      | CF, | CG,  | CI, |
|        |                     | CM, | GΑ, | GN,         | GW,         | ML,       | MR,            | NE,             | SN,             | TD,  | ΤG   |          |     |          |     |      |     |
| CA     | CA 2319807          |     |     | A1          | A1 19990812 |           |                | CA 1999-2319807 |                 |      |      | 19990208 |     |          |     |      |     |
|        | AU 9924398          |     |     |             |             |           | AU 1999-24398  |                 |                 |      |      | 19990208 |     |          |     |      |     |
|        | 7510                |     |     |             |             |           |                |                 |                 |      |      |          |     |          |     |      |     |
| EP     | EP 1054011          |     |     | A1 20001122 |             |           | EP 1999-903901 |                 |                 |      |      | 19990208 |     |          |     |      |     |
| EP     | 1054                |     |     |             |             |           |                |                 |                 |      |      |          |     |          |     |      |     |
|        | R:                  | ΑT, | BE, | CH,         | DE,         | DK,       | ES,            | FR,             | GB,             | GR,  | ΙT,  | LI,      | LU, | NL,      | SE, | MC,  | PT, |
|        |                     | ΙE, | FI, | CY          |             |           |                |                 |                 |      |      |          |     |          |     |      |     |
| NZ     | NZ 506249           |     |     |             | A 20030429  |           |                | NZ 1999-506249  |                 |      |      |          |     |          |     |      |     |
| AT     | AT 339410           |     |     |             | T 200610    |           |                | 1015            | AT 1999-903901  |      |      |          |     | 19990208 |     |      |     |
| RIORIT | ORITY APPLN. INFO.: |     |     |             |             |           |                |                 |                 | JP 1 |      |          |     |          |     |      |     |
|        |                     |     |     |             |             |           |                |                 |                 | WO 1 | 999- | JP54:    | 1   | 1        | W 1 | 9990 | 208 |
| THER S | HER SOURCE(S):      |     |     |             | MAR         | PAT       | 131:           | 1298            | 25              |      |      |          |     |          |     |      |     |

The title compds. [I; R1 = iso-Bu, tigloyl, isovaleryl, 2-methylbutanoyl; R2 = H, aromatic acyl, protecting group such substituted benzoyl, substituted nicotinoyl; R3 = H, nitro, amino, acylamino, N,N-dialkylamino; with provisos] are prepared Thus, UK-2A in CH2Cl2 containing pyridine and PCl5 was refluxed for 1.5 h, the reaction mixture was allowed to cool and then reacted with methanol for 15 h to give (2R,3R,4S,7S)-7-amino-2-benzyl-5,9-dioxa-3-isobutyryloxy-4-methyl-1,6-cyclononanedione. In an antifungal test, (2R,3R,4S,7S)-7-(2-hydroxynicotinylamino)-2-benzyl-5,9-dioxa-3-isobutyryl-4-methyl-1,6-cyclononanedione (also prepared) at 0.05 μg showed potency almost double that of UK-2A against Saccharomyces cerevisiae.

RN 234112-85-7 HCAPLUS

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[4,6-dimethoxy-3-(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Ι

Absolute stereochemistry.

RN 234112-86-8 HCAPLUS
CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[4,5-dimethoxy-3-(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-

(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

234112-88-0 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4,5-dimethoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

234112-89-1 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[4-methoxy-3-(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-CN dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

234112-90-4 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[4-methoxy-1-oxido-3-CN (phenylmethoxy)-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-

Updated Search

(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-05-4 HCAPLUS

CN Heptanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-06-5 HCAPLUS

CN Decanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-14-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxy-3-nitrobenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-ylester (9CI) (CA INDEX NAME)

RN 234113-15-6 HCAPLUS

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(3-amino-2-hydroxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-16-7 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxy-5-nitrobenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-ylester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-17-8 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(5-amino-2-hydroxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 234113-21-4 HCAPLUS
CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxy-3,5-dinitrobenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

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210300-07-5P 215798-04-2P 215798-05-3P
IT
     234112-77-7P 234112-78-8P 234112-79-9P
     234112-80-2P 234112-81-3P 234112-82-4P
     234112-83-5P 234112-84-6P 234112-87-9P
     234112-91-5P 234112-92-6P 234112-93-7P
     234112-94-8P 234112-95-9P 234112-96-0P
     234112-97-1P 234112-98-2P 234112-99-3P
     234113-00-9P 234113-01-0P 234113-02-1P
     234113-03-2P 234113-04-3P 234113-07-6P
     234113-08-7P 234113-09-8P 234113-10-1P
     234113-11-2P 234113-12-3P 234113-13-4P
     234113-18-9P 234113-19-0P 234113-20-3P
     234113-22-5P 234113-23-6P 234113-24-7P
     234113-25-8P 234113-30-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); IMF (Industrial manufacture); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); USES (Uses)
        (preparation of UK-2A derivs. as antifungals)
     210300-07-5 HCAPLUS
RN
     Propanoic acid, 2-methyl-, (3S,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-
CN
     (phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)
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RN 215798-04-2 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 215798-05-3 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxy-3-methoxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 234112-77-7 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,9R)-3-amino-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 210300-07-5 CMF C19 H25 N O6

Absolute stereochemistry.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 234112-78-8 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-6-methyl-4,9-dioxo-3[[(phenylmethoxy)carbonyl]amino]-8-(phenylmethyl)-1,5-dioxonan-7-yl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-79-9 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(1,2-dihydro-2-oxo-3-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 234112-80-2 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(1,6-dihydro-6-oxo-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-81-3 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-6-methyl-4,9-dioxo-8-(phenylmethyl)-3-[[(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)carbonyl]amino]-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-82-4 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-2-methyl-4-quinolinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-83-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3,4-dihydro-3-oxo-2-quinoxalinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-84-6 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(1,6-dihydro-3-hydroxy-6-oxo-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-87-9 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4,6-dimethoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-91-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[6-(acetyloxy)-4-methoxy-3-(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-92-6 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-6-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 234112-93-7 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[3-(acetyloxy)-4-methoxy-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-94-8 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[3-(benzoyloxy)-4-methoxy-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-95-9 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[4-methoxy-3-[[(1-methylethoxy)carbonyl]oxy]-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Updated Search

RN 234112-96-0 HCAPLUS

CN Butanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-97-1 HCAPLUS

CN Butanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234112-98-2 HCAPLUS

CN Pentanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl methyl ester (9CI) (CA INDEX NAME)

RN 234112-99-3 HCAPLUS

CN Hexanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-00-9 HCAPLUS

CN Heptanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-01-0 HCAPLUS

CN Nonanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl methyl ester (9CI) (CA INDEX NAME)

RN 234113-02-1 HCAPLUS

CN Decanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-03-2 HCAPLUS

CN Pentanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-04-3 HCAPLUS

CN Hexanedioic acid, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl phenylmethyl ester (9CI) (CA INDEX NAME)

RN 234113-07-6 HCAPLUS

CN Pentanedioic acid, butyl 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-08-7 HCAPLUS

CN Heptanedioic acid, mono[4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-09-8 HCAPLUS

CN Decanedioic acid, mono[4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl] ester (9CI) (CA INDEX NAME)

RN 234113-10-1 HCAPLUS

CN Alanine, N-[(phenylmethoxy)carbonyl]-, 4-methoxy-2-[[[(3S,7R,8R,9S)-9-methyl-8-(2-methyl-1-oxopropoxy)-2,6-dioxo-7-(phenylmethyl)-1,5-dioxonan-3-yl]amino]carbonyl]-3-pyridinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-11-2 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[3-[[bis(phenylmethoxy)phosphinyl]oxy]-4-methoxy-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-12-3 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[3-[(diethoxyphosphinyl)oxy]-4-methoxy-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 234113-13-4 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-18-9 HCAPLUS

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(4-chloro-2-hydroxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-19-0 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(5-chloro-2-hydroxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 234113-20-3 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(2-hydroxy-4-methoxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-22-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(dimethylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-23-6 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[5-(dimethylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 234113-24-7 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[(3,5-diamino-2-hydroxybenzoyl)amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-25-8 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[5-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234113-30-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[[1,6-dihydro-4-methoxy-6-oxo-3-(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

167173-85-5, (+)-UK-2A ΙT

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of UK-2A derivs. as antifungals)

167173-85-5 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-4-methoxy-2-metCN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 4 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2007 ACS on STN ANSWER 3 OF 4

1999:184083 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

130:193104

TITLE:

Rice blast controlling agents and wheat scab

INVENTOR(S):

controlling agents

Teraoka, Takeshi; Kuzuhara, Kikuko; Mikoshiba, Haruki; Matsumoto, Kuniomi; Iinuma, Katsuharu; Futamura,

Takafumi; Yasutake, Tetsuya; Sakanaka, Osamu ; Mitomo, Koichi; Taniguchi, Makoto

PATENT ASSIGNEE(S):

Meiji Seika Kaisha, Ltd., Japan

SOURCE:

PCT Int. Appl., 24 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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APPLICATION NO.
                                                                    DATE
                         KIND
                                DATE
    PATENT NO.
                                                                    19980831
                                19990311
                                            WO 1998-JP3876
                         A1
    WO 9911127
        W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
            DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG,
            KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO,
            NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA,
             UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
             CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                            AU 1998-88878
                                19990322
                                                                    19980831
    AU 9888878
                          Α
                                            EP 1998-940634
                                                                    19980831
                          A1
                                20000628
    EP 1013169
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
                                            JP 1997-233658
                                                                 Α
                                                                    19970829
PRIORITY APPLN. INFO.:
                                            WO 1998-JP3876
                                                                 W
                                                                    19980831
                         MARPAT 130:193104
OTHER SOURCE(S):
GΙ
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7-yl ester (9CI) (CA INDEX NAME)

These agents contain a compound represented by formula (I) in which R1 AΒ represents alkyl or alkenyl and R2 represents hydrogen or methoxy. The compound is highly effective in preventing rice blast and wheat scab and is not injurious to the plants. Specific compds. used in the examples are obtained by the method described in a publication presented earlier. Activities of I where R1 = iso-Pr and R2 = H (1), R1 = iso-Pr and R2 = OMe(2), R1 = (Z)-2-butenyl and R2 = OMe(3), R1 = iso-Bu and R2 = OMe(4), and R1 = sec-Bu and R2 = OMe (5), were demonstrated. 167173-87-7 167173-88-8 220766-86-9 IT 220766-87-0 220827-77-0 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses) (as rice blast controlling agents and wheat scab controlling agents) RN167173-87-7 HCAPLUS Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-methoCN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-

Ι

Absolute stereochemistry.

RN 167173-88-8 HCAPLUS

CN Butanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Currently available stereo shown.

RN 220766-86-9 HCAPLUS

CN Propanoic acid, 2-methyl-, 3-[[(3-hydroxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 220766-87-0 HCAPLUS

CN Propanoic acid, 2-methyl-, 3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ i-\text{Pr}-\text{C}-\text{O} & & \text{Me} \\ \hline Ph-\text{CH}_2 & & & O & O & OH \\ \hline & & & & \text{OMe} \\ \hline \end{array}$$

220827-77-0 HCAPLUS RN

3-Pentenoic acid, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (3Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2007 ACS on STN ANSWER 4 OF 4

3

ACCESSION NUMBER:

1999:19692 HCAPLUS

DOCUMENT NUMBER:

130:168617

TITLE:

UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02 III. Absolute configuration of an antifungal antibiotic, UK-2A, and consideration of

its conformation

AUTHOR(S):

Shibata, Kozo; Hanafi, Muhammad; Fujii, Jyunko;

Sakanaka, Osamu; Iinuma, Katsuharu; Ueki,

Masashi; Taniguchi, Makoto

CORPORATE SOURCE:

Faculty of Science, Osaka City University, Osaka,

558-8585, Japan

SOURCE:

Journal of Antibiotics (1998), 51(12), 1113-1116

CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER:

Japan Antibiotics Research Association

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GΙ

The absolute configuration of UK-2A (I) was determined by the elucidation of AΒ the

absolute configurations of butanolide II and the serine derivative III, the products of alkaline hydrolysis of I. The absolute configuration of UK-2A was

Ι

found to be (+)-(2R,3R,4S,7S). 167173-86-6, UK 2B 167173-87-7, UK 2C 167173-88-8, UK 2D IΤ

RL: MSC (Miscellaneous)

(determination of the absolute configuration of UK-2A, an antifungal antibiotic)

167173-86-6 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

167173-87-7 HCAPLUS RN

Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-methoCN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

RN 167173-88-8 HCAPLUS

CN Butanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Currently available stereo shown.

IT 167173-85-5

RL: PRP (Properties)

(determination of the absolute configuration of UK-2A, an antifungal antibiotic)

RN 167173-85-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

6

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 14:26:42 ON 21 MAR 2007)

FILE 'REGISTRY' ENTERED AT 14:26:53 ON 21 MAR 2007

L1 STRUCTURE UPLOADED

L2 14 S L1

L3 277 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:39:46 ON 21 MAR 2007

L4 25 S L3

L5 4 S L4 AND SAKANAKA, O?/AU

=> s 14 not 15

L6 21 L4 NOT L5

=> s 16 and mitomo, k?/au 43 MITOMO, K?/AU

L7 0 L6 AND MITOMO, K?/AU

=> s 16 and tamura, t?/au 5413 TAMURA, T?/AU

L8 0 L6 AND TAMURA, T?/AU

=> s 16 and muraj, y?/au

0 MURAJ, Y?/AU

L9 0 L6 AND MURAJ, Y?/AU

=> s 16 and iinuma, k?/au 395 IINUMA, K?/AU

L10 0 L6 AND IINUMA, K?/AU

=> s 16 and teraoka, t?/au 391 TERAOKA, T?/AU

L11 0 L6 AND TERAOKA, T?/AU

=> s 16 and kuzuhara, k?/au 71 KUZUHARA, K?/AU

L12 0 L6 AND KUZUHARA, K?/AU

=> s 16 and mikoshiba, h?/au

L13 0 L6 AND MIKOSHIBA, H?/AU

163 MIKOSHIBA, H?/AU

L14 12 L6 AND TANIGUCHI, M?/AU

=> d 114, ibib abs hitstr, 1-12

L14 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:453925 HCAPLUS

DOCUMENT NUMBER:

145:76021

TITLE:

Structure-activity relationship studies on UK-2A, a novel antifungal antibiotic from Streptomyces sp.

517-02. Part 5: Roles of the 9-membered dilactone-ring

moiety in respiratory inhibition

AUTHOR(S): Usuki, Yoshinosuke; Adachi, Noriko; Fujita, Ken-Ichi;

Ichimura, Akio; Iio, Hideo; Taniguchi, Makoto

CORPORATE SOURCE:

Department of Material Science, Graduate School of

Science, Osaka City University, 3-3-138 Sugimoto,

Sumiyoshi, Osaka, 558-8585, Japan

SOURCE:

Bioorganic & Medicinal Chemistry Letters (2006),

16(12), 3319-3322 CODEN: BMCLE8; ISSN: 0960-894X

Elsevier B.V.

PUBLISHER: DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 145:76021

Several open-chained analogs of UK-2A, a novel antifungal antibiotic isolated from Streptomyces sp. 517-02, were prepared for structure-activity studies. The in vitro antifungal activities of these compds. against Rhodotorula mucilaginosa IFO 0001 and the inhibition of uncoupler-stimulated respiration in bovine heart submitochondrial particles (SMP) were evaluated. Oxidative potentials were measured by cyclic voltammetry. An analog prepared from dihexyl -glutamate showed comparable inhibitory activity as UK-2A.

167173-85-5DP, UK-2A, analogs TT

RL: DMA (Drug mechanism of action); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(SAR of and preparation antifungal UK-2A analogs: 9-membered dilactone-ring moiety role in respiratory inhibition)

167173-85-5 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS 19 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2007 ACS on STN L14 ANSWER 2 OF 12

ACCESSION NUMBER:

2004:937345 HCAPLUS

DOCUMENT NUMBER:

142:348094

TITLE:

UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02 VI (3). Role of substituents on dilactone ring of UK-2A and antimycin A3 against generation of reactive oxygen species in porcine renal

proximal tubule LLC-PK1 cells.

AUTHOR (S):

Fujita, Ken-Ichi; Kiso, Tetsuo; Usuki, Yoshinosuke;

Tanaka, Toshio; Taniguchi, Makoto

CORPORATE SOURCE:

Graduate School of Science, Osaka City University,

Osaka, 558-8585, Japan

SOURCE:

Journal of Antibiotics (2004), 57(10), 687-690

CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER: Japan Antibiotics Research Association

DOCUMENT TYPE: Journal LANGUAGE: English

The role of the substituents on the dilactone of UK-2A and antimycin A3 (AA) against reactive oxygen species (ROS) generation in porcine renal proximal tubule LLC-PK1 cells was studied. Results showed that AA and its derivs. 4~7 stimulated ROS generation. They have a 3-formamidosalicylic moiety at the C7 position. The level of ROS generation induced by AA at 5 and 10 μM were the highest among the derivs. tested and 2.3-fold of the control. On the other hand, UK-2A and its derivs. 1~3, epi-1 and epi-2 did not greatly stimulate ROS generation. These results indicate that a 3-formamidosalicylic moiety contributes to ROS generation. In addition, the level of ROS generation among the derivs. correlated with the intensity of respiratory inhibition. The LLC-PK1 cells treated with the derivs. tested in this study showed morphologies similar to necrotic cell death under microscopic observation. However, it has been reported that AA induces the activation of caspases and DNA fragmentation, which are typical apoptotic responses.

IT 167173-85-5, UK-2A 167173-87-7 215798-04-2

464157-53-7 464157-56-0

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp.)

RN 167173-85-5 HCAPLUS

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-vl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 167173-87-7 HCAPLUS

CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 215798-04-2 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 464157-53-7 HCAPLUS

CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 464157-56-0 HCAPLUS

CN Butanoic acid, 3-methyl-, (3R,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2002:508203 HCAPLUS

DOCUMENT NUMBER:

137:279002

TITLE:

UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02 VI (2). Structure-activity

relationships of UK-2A

AUTHOR(S):

Usuki, Yoshinosuke; Goto, Kimihiko; Kiso, Tetsuo; Tani, Kazunori; Ping, Xu; Fujita, Ken-Ichi; Iio,

Hideo; Taniguchi, Makoto

CORPORATE SOURCE:

Graduate School of Science, Osaka City University,

Osaka, 558-8585, Japan

SOURCE:

Journal of Antibiotics (2002), 55(6), 607-610

CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER:

Japan Antibiotics Research Association

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GΙ

AB UK-2A and antimycin A3 analogs, e.g. I, were tested for their respiratory inhibition in bovine heart SMP and their cytotoxic activity was measured against porcine renal proximal tubule cells. The structure activity relationship was examined as well.

IT 167173-85-5, UK-2A 167173-87-7 215798-04-2 "

464157-53-7 464157-56-0

RL: BSÜ (Biological study, unclassified); BIOL (Biological study) (respiratory inhibition, cytotoxicity, and structure-activity relationships of UK-2A and antimycin A3 synthetic hybrids)

RN 167173-85-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 167173-87-7 HCAPLUS

CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 215798-04-2 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 464157-53-7 HCAPLUS

CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[3-(formylamino)-2-hydroxybenzoyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Updated Search

RN 464157-56-0 HCAPLUS

CN Butanoic acid, 3-methyl-, (3R,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2002:262139 HCAPLUS

DOCUMENT NUMBER:

137:30441

TITLE:

UK-2A, B, C, and D, novel antifungal antibiotics from Streptomyces sp. 517-02: VII. Membrane injury induced by C9-UK-2A, a derivative of UK-2A, in Rhodotorula

mucilaginosa IFO 0001

AUTHOR(S):

Tani, Kazunori; Usuki, Yoshinosuke; Motoba, Kazuhiko;

Fujita, Ken-Ichi; Taniguchi, Makoto

CORPORATE SOURCE:

Graduate School of Science, Osaka City University,

Osaka, 558-8585, Japan

SOURCE:

Journal of Antibiotics (2002), 55(3), 315-321

CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER:

Japan Antibiotics Research Association

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

UK-2A is a potent antifungal antibiotic and its structure is highly AB similar to that of antimycin A3 (AA). UK-2A and AA inhibit mitochondrial electron transport at complex III. However, the antifungal activities of UK-2A and AA disappear after 48-h treatment. In an attempt to improve the duration of the antifungal activity of UK-2A, several UK-2A derivs. were prepared by substituting its nine-membered dilactone ring with an n-alkyl or an isoprenyl moiety. Among all the derivs. tested, C9-UK-2A (I) and C10-UK-2A showed the most potent and durable antifungal activities against a strict aerobic yeast, Rhodotorula mucilaginosa IFO 0001. I, in particular, continued to demonstrate its broad-spectrum antifungal activity after 120-h treatment. Therefore, we focused on I to further examine its mode of action against the yeast. Interestingly, I did not inhibit cellular respiration of the cells even at concns. greater than 100  $\mu g/mL$  . I gradually induced the efflux of potassium ions from the cells. Moreover, I gradually induced the release of glucose from glucose-encapsulating liposomes. The patterns of efflux and release induced by I were not as rapid as those seen with amphotericin B. These results suggest a membrane injury caused by I in R. mucilaginosa IFO 0001.

IT 167173-85-5, UK-2A
RL: PAC (Pharmacological activity); BIOL (Biological study)
(activity of UK-2A and derivs. against Rhodotorula mucilaginosa)

RN 167173-85-5 HCAPLUS

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:557166 HCAPLUS

DOCUMENT NUMBER: 135:300904

TITLE: UK-2A, B, C and D, novel antifungal antibiotics from

Streptomyces sp. 517-02. VI (1). Structure-activity

relationships of UK-2A

AUTHOR(S): Usuki, Yoshinosuke; Tani, Kazunori; Fujita, Ken-Ichi;

Taniguchi, Makoto

CORPORATE SOURCE:

Graduate School of Science, Osaka City University,

Osaka, 558-8585, Japan

SOURCE:

Journal of Antibiotics (2001), 54(7), 600-602

CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER:

Japan Antibiotics Research Association

DOCUMENT TYPE: Journal LANGUAGE: English

The synthesis of UK-2A analogs, where the nine-membered dilactone residue AΒ was replaced by several alkyl or isoprenyl moieties, and their biol. effects were studied. All the tested compds., such as UK-2A, AA, and their derivs., did not show any growth inhibitory activity against both Gram-neg. and Gram-pos. bacteria up to  $100 \, \mu g/mL$ . Salicylic acid moiety or pyridinecarboxylic acid moiety plus a hydrophobic structure is at least necessary for expression of antifungal action. The 9-membered dilactone ring moiety itself is not essential for the antimicrobial activity, and C8-alkyl group is flexible and hydrophobic that makes C8-UK-2A interact the binding domain to prevent yeasts and filamentous fungi from growing. The decrease in activity of isoprenylated UK-2A derivs. was due to a loss of flexibility, which interferes in their taking active conformations. AA had strong cytotoxicity against porcine renal proximal tubule LLC-PK1 cells and other types of cultured cells compared to UK-2A. The inhibitory of UK-2A and AA for the uncoupler stimulated respiration of bovine heart submitochondrial particles was examined C8-3MeOSA showed comparably high inhibitory activity similar to C8-AA and AA, although its antimicrobial activities were weaker than those were. The mode of action of C8-UK-2A would be different from that of UK-2A.

IT 167173-85-5, UK-2A

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02. VI (1). Structure-activity relationships of UK-2A)

RN 167173-85-5 HCAPLUS

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1999:574605 HCAPLUS

DOCUMENT NUMBER:

131:297409

TITLE:

UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02 V. Inhibition mechanism of

bovine heart mitochondrial cytochrome bcl by the novel

antibiotic UK-2A

AUTHOR(S):

SOURCE:

Machida, Kiyotaka; Takimoto, Hiroaki; Miyoshi, Hideto;

Taniguchi, Makoto

CORPORATE SOURCE:

Department of Biology, Graduate School of Science,

Osaka City University, Osaka, 558-8585, Japan Journal of Antibiotics (1999), 52(8), 748-753

CODEN: JANTAJ; ISSN: 0021-8820

Japan Antibiotics Research Association PUBLISHER:

DOCUMENT TYPE:

Journal English LANGUAGE:

UK-2A is a potent antifungal antibiotic isolated from Streptomyces sp. AΒ 517-02 and its structure is highly similar to that of antimycin A. authors investigated the inhibition mechanism of bovine heart mitochondrial cytochrome bc1 complex by the UK-2A using antimycin A and myxothiazol as the reference inhibitors of ubiquinol oxidation (Qo) and

ubiquinone

reduction (Qi) sites, resp. The inhibitory potency of UK-2A was about 3-fold less than antimycin A. On the basis of the effects of UK-2A on the reduction kinetics of b and c1 hemes, this compound appeared to be an inhibitor of the Qi site. However, since spectral changes of dithionite-reduced cytochrome b induced by UK-2A binding differed from that of antimycin A, the precise binding manner of UK-2A to the enzyme is not identical to that of antimycin A. It could be concluded that antimycin A binding to cytochrome b is primarily decided by structural specificity of the salicylic acid moiety.

167173-85-5, Antibiotic UK-2A 167173-86-6, Antibiotic ΙT UK-2B 167173-87-7, Antibiotic UK-2C 167173-88-8, Antibiotic UK-2D

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(UK-2A, B, C and D as novel antifungal antibiotics from Streptomyces)

167173-85-5 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

167173-86-6 HCAPLUS RN

2-Butenoic acid, 2-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-4-methoxy-2-CN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 167173-87-7 HCAPLUS

CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 167173-88-8 HCAPLUS

CN Butanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Currently available stereo shown.

REFERENCE COUNT:

THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1999:368241 HCAPLUS

DOCUMENT NUMBER:

131:125082

TITLE:

UK-2A, B, C and D, novel antifungal antibiotics from

Updated Search

AUTHOR(S):

SOURCE:

Streptomyces sp. 517-02: IV. Comparative studies of UK-2A with antimycin A3 on cytotoxic activity and reactive oxygen species generation in LLC-PK1 cells

Takimoto, Hiroaki; Machida, Kiyotaka; Ueki, Masashi;

Tanaka, Toshio; Taniguchi, Makoto

CORPORATE SOURCE: Department of Biology, Graduate School of Science,

Osaka City University, Osaka, 558-8585, Japan Journal of Antibiotics (1999), 52(5), 480-484

CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER: Japan Antibiotics Research Association

DOCUMENT TYPE: Journal LANGUAGE: English

AB UK-2A, a novel antifungal antibiotic, is a structural relative of antimycin A3 (AA) and its mode of action is similar to that of AA which inhibits mitochondrial electron transport at complex III. In spite of their structural resemblance, AA had strong cytotoxicity while UK-2A had little cytotoxicity against LLC-PK1 cells as well as other types of cultured cells. When cells were treated with UK-2A or with AA the intracellular ATP content decreased significantly within 5 min in glucose-free medium to almost the same extent in both cases. Moreover, under the same conditions, UK-2A killed cells at a similar rate to AA. This suggested that UK-2A entered into the cells and, like AA, inhibited mitochondrial electron transport. On the other hand, AA stimulated reactive oxygen species (ROS) production within 5 min even at a low

concentration of 1  $\mu M$  whereas UK-2A did not show such an effect. The difference in the ROS-producing abilities of UK-2A and AA may account for the different cytotoxic effects of the two compds.

IT 167173-85-5, UK-2A

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(comparative studies of UK-2A with antimycin A3 on cytotoxic activity and reactive oxygen species generation in LLC-PK1 cells)

RN 167173-85-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:22846 HCAPLUS

DOCUMENT NUMBER: 128:163891

TITLE:

The mode of action of UK-2A and UK-3A, novel

antifungal antibiotics from Streptomyces sp. 517-02

Ueki, Masashi; Taniguchi, Makoto AUTHOR(S):

CORPORATE SOURCE:

Dep. Biology, Fac. Sci., Osaka City Univ., Osaka, 558,

Japan

SOURCE:

Journal of Antibiotics (1997), 50(12), 1052-1057

CODEN: JANTAJ; ISSN: 0021-8820

PUBLISHER:

Japan Antibiotics Research Association

DOCUMENT TYPE:

Journal

LANGUAGE:

English

UK-2A and UK-3A are structural relatives of antimycins, which were AB isolated as antifungal antibiotics with little cytotoxicity that demonstrated inhibition of respiratory activity. They halve the cellular respiration of yeast within 4~5 min and the intracellular ATP content within 2~5 min. They inhibited the yeast mitochondrial respiration using  $\beta$ -hydroxybutyrate and succinate as a respiratory substrate, but no inhibition was observed using ascorbate-reduced tetra-Me p-phenylenediamine as the substrate. The site of respiratory inhibition of UK-2A and UK-3A was thought to be the cytochrome bcl complex in the mitochondrial electron transport chain of yeast cells. They also inhibited the mitochondrial respiration of rat liver. Intact animal cells might have some system to defend themselves from the actions of UK-2A and UK-3A.

167173-85-5, UK-2A 194931-82-3, Antibiotic UK-3A IT RL: BUU (Biological use, unclassified); BIOL (Biological study); USES

(mechanism of antifungal action of UK-2A and UK-3A)

167173-85-5 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S, 6S, 7R, 8R)-3-[[(3-hydroxy-4-methoxy-2-metCN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 194931-82-3 HCAPLUS

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-2-CN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS 16 ' RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2007 ACS on STN L14 ANSWER 9 OF 12

1997:504110 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 127:217524

UK-3A, a novel antifungal antibiotic from Streptomyces TITLE:

sp. 517-02: fermentation, isolation, structural

elucidation and biological properties

Ueki, Masashi; Kusumoto, Atsushi; Hanafi, Muhammad; AUTHOR(S):

Shibata, Kozo; Tanaka, Toshio; Taniguchi,

Makoto

Faculty of Science, Osaka City University, Osaka, 558, CORPORATE SOURCE:

Japan

Journal of Antibiotics (1997), 50(7), 551-555 SOURCE:

CODEN: JANTAJ; ISSN: 0021-8820

Japan Antibiotics Research Association PUBLISHER:

Journal DOCUMENT TYPE:

English LANGUAGE:

GI

A novel antifungal antibiotic, UK-3A (I), was obtained from the mycelial AΒ cake of Streptomyces sp. 517-02. I was very similar in structure to UK-2A, a structural relative of antimycin A. The antifungal spectrum of I was relatively broad (MICs for yeasts and filamentous fungi: 1.56.apprx.6.25 and 0.39.apprx.1.56  $\mu$ g/mL, resp.). The cytotoxic activity of I was weak (IC50: 18.apprx.100  $\mu$ g/mL).

194931-82-3P, Antibiotic UK 3A RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BPN (Biosynthetic preparation); BSU (Biological study,

unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (UK-3A is a novel antifungal antibiotic from Streptomyces) 194931-82-3 HCAPLUS RN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-2-CN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

1997:16443 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 126:144017

UK-2A, B, C and D, novel antifungal antibiotics from TITLE:

Streptomyces sp. 517-02. II. Structural elucidation

Hanafi, Muhammad; Shibata, Kozo; Ueki, Masashi; AUTHOR(S):

Taniguchi, Makoto

CORPORATE SOURCE:

Fac. Sci., Osaka City Univ., Osaka, 558, Japan Journal of Antibiotics (1996), 49(12), 1226-1231 SOURCE:

CODEN: JANTAJ; ISSN: 0021-8820

Japan Antibiotics Research Association PUBLISHER:

Journal DOCUMENT TYPE: English LANGUAGE:

UK-2A, UK-2B, UK-2C and UK-2D, novel antibiotics produced by Streptomyces AΒ sp. 517-02, exhibit strong antifungal activity. The structures were

elucidated based on spectral and chemical evidence that these compds. are the

derivs. of the nine-membered dilactone formed from serine and 4-hydroxypentanoic acid moiety.

167173-86-6P 167173-87-7P, UK 2C 167173-88-8P, TΤ

RL: PRP (Properties); PUR (Purification or recovery); PREP (Preparation) (structural elucidation of UK-2A, UK-2B, UK-2C and UK-2D, novel antifungal antibiotics from Streptomyces sp. 517-02)

167173-86-6 HCAPLUS RN

2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 167173-87-7 HCAPLUS

CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 167173-88-8 HCAPLUS

CN Butanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Currently available stereo shown.

IT 167173-85-5P

RL: PRP (Properties); PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (structural elucidation of UK-2A, UK-2B, UK-2C and UK-2D, novel antifungal antibiotics from Streptomyces sp. 517-02)

RN 167173-85-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-

(CA INDEX NAME) 7-yl ester (9CI)

Rotation (+). Absolute stereochemistry.

186528-19-8P, O-Methyl UK 2A IT

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (structural elucidation of UK-2A, UK-2B, UK-2C and UK-2D, novel antifungal antibiotics from Streptomyces sp. 517-02)

186528-19-8 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3,4-dimethoxy-2-CN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2007 ACS on STN L14 ANSWER 11 OF 12

ACCESSION NUMBER: 1996:463922 HCAPLUS

DOCUMENT NUMBER: 125:109869

TITLE: UK-2A, B, C and D, novel antifungal antibiotics from

Streptomyces sp. 517-02. I. Fermentation, isolation,

and biological properties

Ueki, Masahi; Abe, Keiichi; Hanafi, Muhammad; Shibata, AUTHOR(S):

Kozo; Tanaka, Toshio; Taniguchi, Makoto Fac. Science, Osaka City Univ., Osaka, 558, Japan CORPORATE SOURCE:

Journal of Antibiotics (1996), 49(7), 639-643 SOURCE:

CODEN: JANTAJ; ISSN: 0021-8820

Japan Antibiotics Research Association PUBLISHER:

Journal DOCUMENT TYPE:

English LANGUAGE:

GΙ

$$CH_2$$
 $O$ 
 $NHCO$ 
 $NHCO$ 
 $I$ 
 $R$  =  $CHMe_2$ 
 $II$ 
 $R$  =  $CH$   $(Me)$  =  $CHMe$ 

AB Novel antifungal antibiotics, UK-2A (I), UK-2B (II) and a mixture of UK-2C and UK-2D, were obtained from the mycelial cake of Streptomyces sp. 517-02. All of the UK-2 compds. were similar in structure to antimycin A. The antifungal activities of of UK-2 compds. were as strong as that of antimycin A. However, the UK-2 compds. demonstrated weak cytotoxicity compared to antimycin A.

IT 167173-85-5, UK 2A 167173-86-6, UK 2B 167173-87-7, UK 2C 167173-88-8, UK 2D RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (UK-2A, B, C and D, novel antifungal antibiotics from Streptomyces sp. 517-02. I. Fermentation, isolation, and biol. properties)

RN 167173-85-5 HCAPLUS

CN Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 167173-86-6 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 167173-87-7 HCAPLUS

CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 167173-88-8 HCAPLUS

CN Butanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Currently available stereo shown.

L14 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:934118 HCAPLUS

DOCUMENT NUMBER: 123:337552

TITLE: Fungicides manufacture with Streptoverticillium

INVENTOR(S): Taniguchi, Makoto; Shibata, Kozo; Abe,

Keiichi; Kodama, Tooru; Uotani, Kazumichi; Oonishi,

Yoshitaka

Suntory Ltd., Japan; Meiji Seika Co.; Meiji Seika PATENT ASSIGNEE(S):

Kaisha, Ltd.

Jpn. Kokai Tokkyo Koho, 10 pp. SOURCE:

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO.                        | KIND    | DATE        | APPLICATION NO. | DATE     |
|-----------------------------------|---------|-------------|-----------------|----------|
| JP 07233165                       | A<br>B2 | 19950905    | JP 1994-26884   | 19940224 |
| JP 3526602 PRIORITY APPLN. INFO.: |         | 123:337552  | JP 1994-26884   | 19940224 |
| OTHER SOURCE(S):                  | HAINEAT | 123.33/1332 |                 |          |

$$\begin{array}{c|c} N & H & O & \\ \hline OH & O & \\ \hline OH & O & \\ \hline \end{array}$$

Fungicides (I: R = linear or branched aliphatic (un)saturated acyl group) are AB manufactured by culturing Streptoverticillium sp. SAM2084. Shake-culture of Streptoverticillium sp. SAM2084 for manufacture of four I wherein R = 2-methylpropanoyl (UK-2A), trans-2-methyl-2-butenoyl (UK-2B), 3-methylbutanoyl (UK-2C), and 2-methylbutanoyl (UK-2D) was shown. Also given were the physiol. and morphol. characteristics of the Streptoverticillium sp. SAM2084.

Ι

167173-85-5P, UK 2A 167173-86-6P, UK 2B ΙT 167173-87-7P, UK 2C 167173-88-8P, UK 2D RL: BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (fungicides manufacture with Streptoverticillium)

167173-85-5 HCAPLUS RN

Propanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-CN pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 167173-86-6 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 167173-87-7 HCAPLUS

CN Butanoic acid, 3-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 167173-88-8 HCAPLUS

CN Butanoic acid, 2-methyl-, (3S,6S,7R,8R)-3-[[(3-hydroxy-4-methoxy-2-pyridinyl)carbonyl]amino]-6-methyl-4,9-dioxo-8-(phenylmethyl)-1,5-dioxonan-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Currently available stereo shown.

\_ ... #

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9
                             13
                                 14
                                     15
                                         16 .17
                                                18
   1 2 3 4
                   7
                       8
                  6
chain bonds :
                                               27-36 29-30 31-32
   1-11 6-10
                           12-15 23-24
                                         23-25
               7-12
                   11-27
ring bonds :
                           5-9 6-7 7-8 8-9 13-14 13-18 14-15 15-16
            2-3
                 3-6
                      4 – 5
   1-2 	 1-4
   16-17
          17-18
exact/norm bonds :
   1-11 6-10 11-27 23-24
                            23-25
                                   27-36
exact bonds :
   1-2 1-4 2-3 3-6 4-5 5-9 6-7 7-8 7-12 8-9 12-15 29-30
                                                                  31 - 32
normalized bonds :
                      15-16 16-17 17-18
   13-14 13-18 14-15
isolated ring systems :
   containing 1 : 13 :
G1:CH3,Et
G2:OH, [*1], [*2]
G3:NH2,NO2,[*3]
Match level :
                  3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
   1:Atom 2:Atom
   10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
   18:Atom 20:CLASS 21:Atom 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom
   29:CLASS 30:CLASS 31:CLASS 32:CLASS 36:CLASS 38:CLASS 39:Atom
   40:CLASS
Generic attributes :
   27:
   Saturation
                         : Unsaturated
```

chain nodes :

ring nodes :

10 11 12

Number of Carbon Atoms : less than 7 Number of Hetero Atoms : Exactly 1 Type of Ring System : Monocyclic

Element Count :

Node 27: Limited C,C5

N,N1

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                 CAS Registry Number crossover limit increased from 10,000
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                 to 300,000 in multiple databases
                 WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 24
        MAR 15
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NEWS 25
        MAR 16
NEWS 26
        MAR 20 MARPAT now updated daily
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L3

O SEA SSS FUL L1

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(Untitled)
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chain nodes :
   7 17 18
ring nodes :
                            11
   1 2 3 4 5 6 8
                      9
                         10
                                12
                                    13
                                        14 15
chain bonds :
   3-7 7-9 15-18 16-17
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-13 12-14 13-16
   14-15 15-16
exact/norm bonds :
   15-18 16-17
exact bonds :
   3-7 7-9 8-9 8-12 9-10 10-11
                                  11-13 12-14 13-16 14-15 15-16
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
   containing 8 :
Match level :
   1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom
   10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS
   18:CLASS
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